Diisopropyl fluorophosphate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.90e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.51e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

Image not found
Triethyl phosphate
Measured: 5.53e-11
Predicted: 4.26e-11

Image not found
Ethyl ethylcarbamate
Measured: 1.44e-11
Predicted: 1.58e-11

Image not found
Dimefox
Measured: 6.40e-11
Predicted: 3.64e-11

Image not found
Phosphoramidic acid, dimethyl-,
dimethyl ester
Measured: 3.19e-11
Predicted: 2.75e-11

Image not found
N-Methylcarbamic acid, ethyl
ester
Measured: 8.30e-12
Predicted: 1.01e-11